Electronic Supporting Information for:

Ring-Oxidized Zinc(II)Phthalocyanine Cations: Structure, Spectroscopy and Decomposition Behavior

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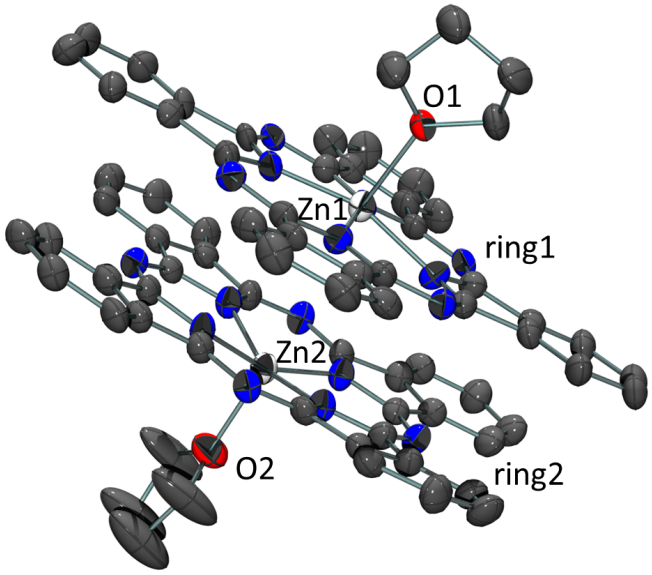

Figure S1: Crystal structure of $[PcZn(C_4H_8O)]^{\bullet}{}_2[Bar^F{}_4]_2$ (**1**•THF) (ring = average plane of inner N_8C_8 ring, $Bar^F{}_4^-$ counter ions excluded for clarity, oxygen: red, nitrogen: blue, carbon: grey). Bond lengths and inter-ligand distances (Å) Zn1-Zn2 3.95(1), Zn1-ring1 0.34(1), Zn2-ring2 0.43(1), ring1-ring2 3.18(1), Zn1-O1 2.10(1), Zn2-O2 2.09(1).

Table S1: Crystallographic data table for **1**•THF.

Compound Reference	Compound **1**
Chemical Formula	$C_{130.5}H_{60}$ B2$F_{40}N_{16}O_2Zn_2$
Formula Mass	2796.31
a/Å	12.8320(9)
b/Å	51.244(4)
c/Å	18.033(1)
α/˚	90
β/˚	97.456(5)
γ/˚	90
Unit cell volume/$Å^3$	11757(2)
Temperature/K	150(2)
Space group	P 21/n
Number of formula unit per cell/Z	4
Radiation type	Cu Kα
Absorption coefficient, μ/mm^{-1}	1.624
No. of reflections	95942
R_{int}	0.0766
Final R_1 values (I>2σ(I))	0.1642
Final wR(F^2) values (I>2σ(I))	0.3573
Final R_1 values (all data)	0.1802
Final wR(F^2) (all data)	0.3657
Goodness of fit	1.213

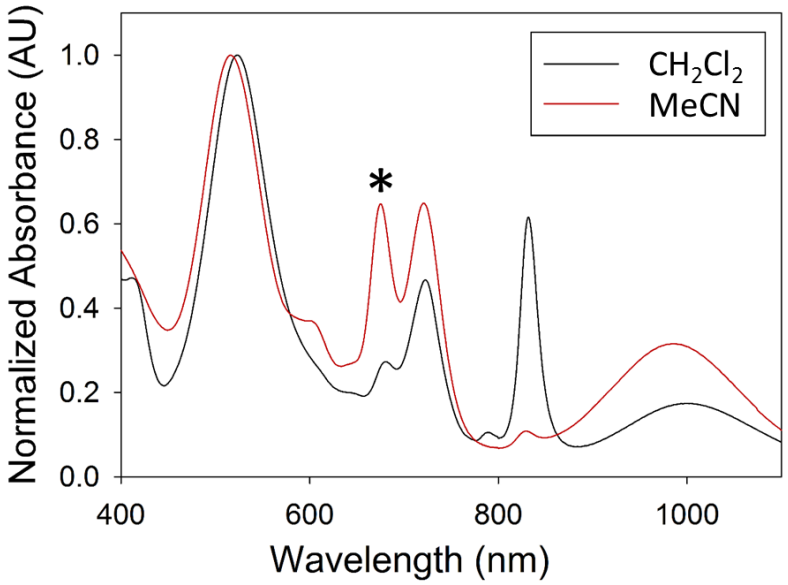

Figure S2: UV-Visible absorption plots for 0.1 mM solutions of **1**•THF in CH_2Cl_2 (black) and MeCN (red) (* marks absorbance maximum of **2** in solution from decomposition of **1**•THF).

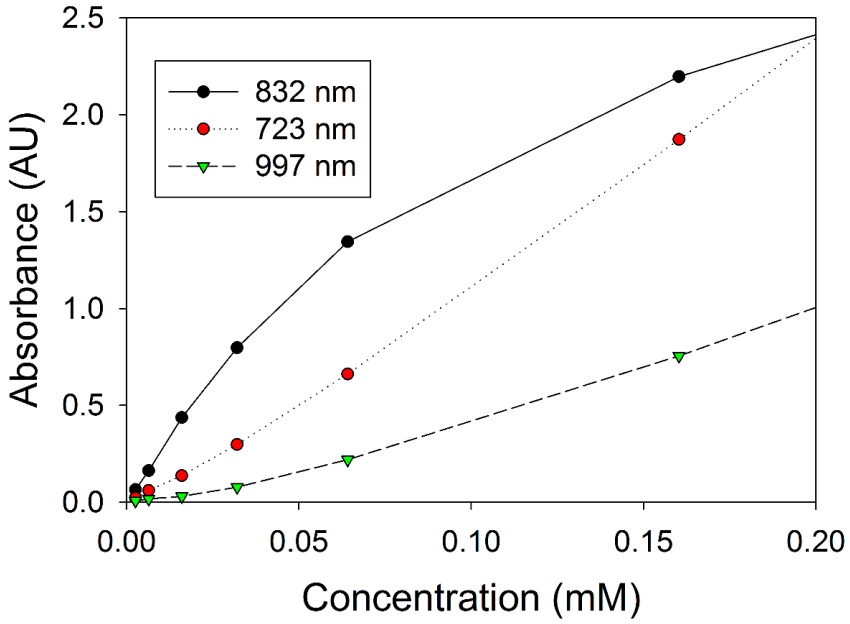

Figure S3: Beer-Lambert plot of compound **1**•THF in CH_2Cl_2.

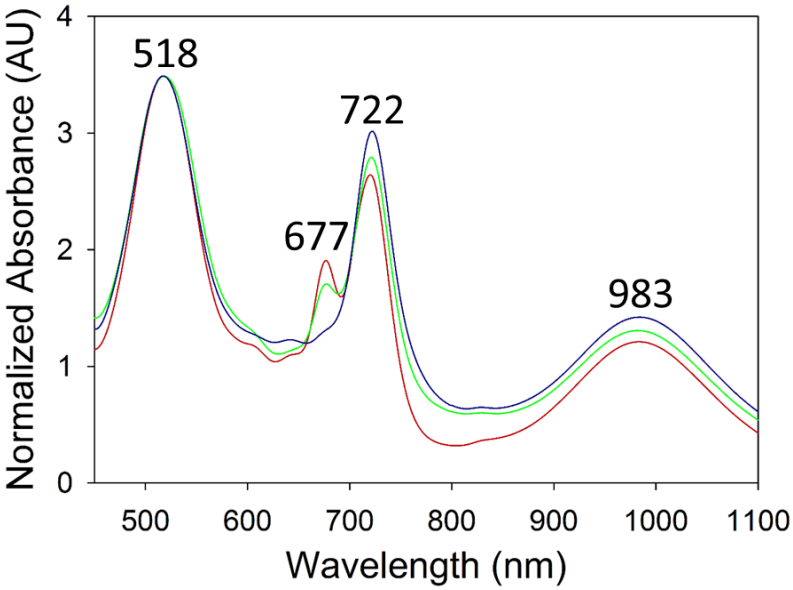

Figure S4: UV-Visible absorption spectrum of a 2.0m M solution of a 1:1 molar ratio mixture of compounds **1**•THF and **2** in MeCN after 5 min (red), 24 h (green) and 96 h (blue) (normalized to the absorption at 518 nm).

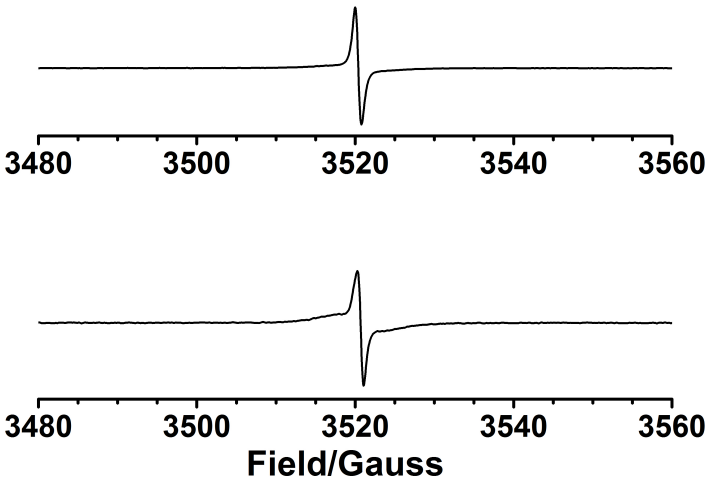

Figure S5: EPR of 1.0mM (top) and 10mM (bottom) solutions of **1**•THF in MeCN.

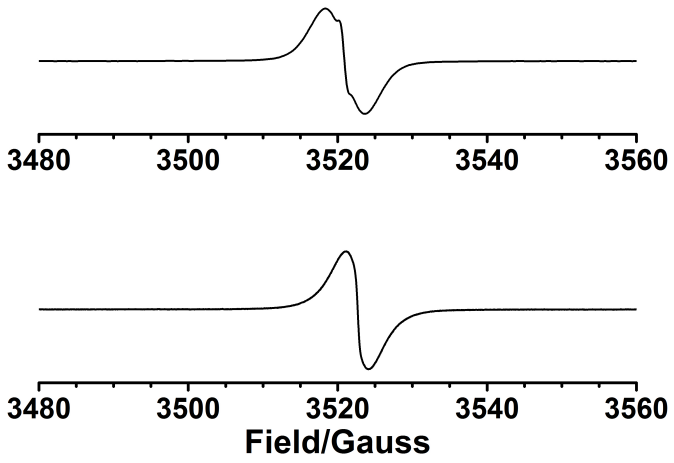

Figure S6: EPR of **1**•THF in CH_2Cl_2 at a concentration of 10 mM (top) and in the solid state (bottom).